

## **$^{13}\text{C}$ NMR chemical shifts and local structure of cis-1,4-polybutadiene: Calculation and experiment**

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### **Abstract**

© 2016, Pleiades Publishing, Ltd. The quantum-chemical modeling of the local conformational structures of a cis-1,4-polybutadiene macromolecule is performed, and the magnetic shielding constants of  $^{13}\text{C}$  nuclei are calculated. The theoretical values of chemical shifts in the  $^{13}\text{C}$  NMR spectra are compared with the corresponding experimental data.

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